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Screened Charge Model in the Treatment of Electrostatic Interactions[1] BO WANG, HANNAH LEVERENTZ, Department of Chemistry, University of Minnesota, DONALD TRUHLAR, Department of Chemistry and Supercomputing Institute, University of Minnesota — Partial atomic charges play an important role in molecular simulations of complex systems, and they are widely used to compute the electrostatic interactions in various methods. We propose a screened charge model to include charge penetration and screening effects in electrostatic modeling. In the screened charge model, the atomic charge density of an atom in a molecule is represented by a spherical smeared charge plus a point charge at the nucleus. The new model is illustrated for the electronically embedded combined quantum mechanical and molecular mechanical (QM/MM) calculations and for the electrostatically embedded many-body (EE-MB) method. For a test set of 40 complexes, the mean unsigned error of QM/MM electrostatic interactions between QM and MM regions is reduced from 8.1 to 2.8 kcal/mol and that for QM/MM induction interactions from 1.9 to 1.4 kcal/mol. In a test of five water hexamers, the mean unsigned error of the EE-MB binding energies of the clusters is decreased by a factor of 2 at both the pairwise additive (PA) and three-body (3B) levels. Moreover, we have found that the charges derived by fitting electrostatic potentials with the screened charge method are less sensitive to the positions of the fitting points, and the quality of the fit to the electrostatics is improved.

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